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Deconvolve: a protocol and R package for thermogravimetric decay curve deconvolution for lignocellulosic biomass trait calculation

(what a mouthful….)

TG/DTG thermogravimetric/differential thermogravimetry

Get terminology straight about “pseudo compoenents”

Nomenclature table?

Could also just frame it as technique for package to do thermogravimetric analysis to determine lignocelluosic ompoasition of biomass—not in traits perspective… == more applicable. To biofuel etc?

Plant litter characteristics are known to be important drivers of plant-soil interactions, particularly litter dynamics during decomposition. [REL TO OTHER ECO SERVICES?]. While litter of any type can become recalcitrant in the soil for a variety of reasons, including the absence of necessary decomposer communities or required environmental conditions, intrinsically chemically complex litter will almost always become recalcitrant. Litter quality, estimated by traits, is related to relative labillity or refractiveness of litter. It has been found to e a dominant driver of decay rate, stronger even than environmental variables (cor et al 2008), trait effects relate not just to leaf but also to root decay rates (freschet a plant eco spe), and across a range of ecosystems. Most of these studies include some method for calculation C fraction of components particularly lignin, which has been found to be a predominant predictor of litter decay (citations).

Why do we need measures of lignocellulosic biomass?

Establishing the composition of species’ lignocellulosic biomass, consisting primarily of hemicellulose, cellulose, and lignin, and hereafter referred to as ‘biomass’, is an important ….

How do we currently measure?

Conventional chemical methods for measuring lignocellulosic biomass sustain a heavy cost – in environmental impact, time, as well as funding. While it is still possible to use these methods to calculate biomass (makkonen, freschet – mult mech, freschet – plant econ), these limitations have undoubtedly reduced the application of biomass measures to ecological research, even in studies where those data (particularly lignin mass) would be relevant (for example to litter decomposition studies; Quested, Albert – Helene, de Vries et al 2012). Other alternatives include liqueid chromatography (HPLC) and Nnear infraref spectroscopy (NIRS) -- (Birouste, and Rovira et al 2008) did NIRS, but also not ideal or widespread because … While the methodology to calculate many other characteristics of plant material have been thoroughly documented in the trait handbook (perez), methods to measure biomass are notably absent. Unavailability of a faster, more affordable measurement technique is limiting not just those fields to which biomass measures would certainly advance, but also restricting easy exploration of other, until now unaccessed, ties between biomass contents and other ecosystem functions. In this paper, we present a viable alternative for biomass calculation using thermogravimetry and mixture modelling, transparent and reproducibly housed in the ‘deconvolve’ package.

Alternative: TGA

1. couple sentence explanation of tga method.
2. How it’s been used in the past for this purpose

Thermogravimetry pyrolyses biomass across a temperature ramp and records the mass remaining at specified intervals. The pyrolysis curve can be described as the sum of the thermal decay curves of the three main components of biomass: hemicellulose, cellulose, and lignin. Deconvolution separates these pyrolytic profiles into three independent reactions, which correspond to pseudo-hemicellulose, pseudo-cellulose, and pseudo-lignin, hereafter referred to as P-HC, P-CL, and P-LG, respectively. These pseudo components do not necessarily correspond to a pure substance, but they refer to mass that thermally degrades in a concrete temperature interval.

In the biofuel field, pyrolytic profiles generated from thermogravimetry are deconvolved into their three independent reactions in order to estimate kinetic parameters for the overall sample \*\*CHECK THIS LIST (Orfao & Figueiredo 2001, Barneto et al 2009, Cai & Liu 2007, Chen et al 2017). It can also be used to estimate mass fractions of these componetns .

Barneto et al 2011 used tga to characterise the lignocellulosic composition of Eucalyptus wood. They foun comparable percent weight contributions as other studies that measured from scratch (Brito et al 2008). Also Orfao et al 1999

This list uses it for biomass?

(Orfao & Figueiredo 2001, Barneto et al 2009, Cai & Liu 2007, Chen et al 2017)

TGA Method USE Barneto et al 2009

This deconvolution is typically conducted using a peak fitting software. Methods are very difficult to replicate without access to the software, and even with access due to under-reporting of model used in peak deconvolution. This R package provides functions to deconvolve a pyrolytic curve, increasing the reproducibility of this work, as well as making this method of biomass approximation more available to ecologists. Thermogravimetry combined with the deconvolve package provides an easy, inexpensive, and standardised alternative to biomass measures.

Labile peak a tlow or medium temperature and a recalcitrant oen at high temperatures. Lignin typically peaks the latest, but a strong peak may not be visible due to overlapping peaks, and because lignin is degraded over such a wide temperature range that the peak is very low (Duguy & Rovira 2010).

Different math models

Cheng et al 2015 (applicability of fs…), Hu et al 2016 (thermo kinetics…) used Fraser-Suzuki.

Sun et al 2015 (kinetic study…) used asymmetric bi-Gaussian

Chen et al 2017 (thermo pyrolysis… ) used asymmetric double sigmoidal

Perejon et al 2011 (kinetic analysis…) compared Gaussian, Lorentzian, Weibull, and Fraser-Suzuki. Found that Lorentzian and Gaussian are not appropriate because inetic curves are asymmetrical. Showne that fs fits any kinetic curve. Is able to fit curves that follow ideal models as well as those that deviate due to inhomogeneity. Recommend using fs for peak deconvolution of complex reaction into individual processes, and then subsequent kinetic analysis.

In this study we used a three-part Frazer-Suzuki function mixture model to separate the curve into three components. .. next comes math part.

A protocol for lignocellulosic biomass calculation using deconvolve

As described more fully in (Windecker et al 2017).

As with leaf traits in Perez, should collect 10 leaf samples of robust, well-grown individuals.

Litter should be pooled and dried and ground to ~ size.

TG analysis

~10-20 mg of sample should be place in the crucible.

N2 atmosphere over a temperature ramp of 30-800 C at 10C/min.

Raw mass loss data imported into the statistical software R.

Deconvolve package

Mass loss rate was calculated by taking the derivative.

After integrating the curves, you have the mixing proportions of each. These can then be modified by the amount of carbon left in the ash sample to calculate mg component per mg dry weight.

Function inputs: lower, upper

* Data were clipped at 120C and at 600C. 120 C effectively standardises to dry weight, as mass loss before that temperature is considered dehydration water loss. Lignocellulosic components are not considered to be lost about about 600. Mass lost after that is typically interacting with volatiles.

Sample Results – this has been implemented in (Windecker et al. xxxx)

Illustrate with a few different materials. Seagrass sample, woody, gramin, forb? Pure cellulose

Discussion

Limitations

* developed using wetland plants
* some of the initial values will not be appropriate for litter that is too different or that needs to be deconvolved into too many other ocmpoennts. Ex. Woody.

Conclusion

Lignocellulosic biomass calculation with TGA is already relatively inexpensive, this package enables its application to be more widespread by improving ease of use and standardising methods for calculation. using this method is a good candidate for more widespread application in the trait literature. In combination with this package, it is now much more accessible to the majority of ecologists. It is also makes this method more transparent and reproducible.

In this study, I examine a novel method in ecology for calculating lignocellulosic biomass using mixture modelling of thermogravimetric analysis (TGA), typical in the biofuel field. I found that TGA coupled with modelling approaches is a rapid, low-cost assessment method that can be used to estimate partitioning of leaf carbon.

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